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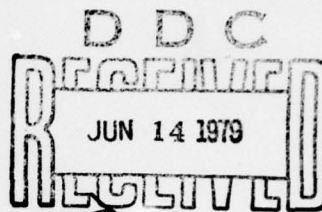
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DESIGN PROBLEMS FOR OPTIMAL SURFACE INTERPOLATION

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## Design problems for optimal surface interpolation

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### ABSTRACT

We consider the problem of interpolating a surface given its values at a finite number of points. We place a special emphasis on the question of choosing the location of the points where the function will be sampled.

Using minimal norm interpolation in reproducing kernel Hilbert spaces, equivalently Bayesian interpolation, and N-widths, we provide lower bounds for interpolation error relative to certain error criteria. These lower bounds can be used when evaluating an existing design, or when attempting to obtain a good design by iterative procedures to decide whether further minimization is worthwhile. The bounds are given in terms of the eigenvalues of a relevant reproducing kernel and the asymptotic behavior of these eigenvalues for certain tensor product spaces in the unit d-dimensional cube is obtained.

We demonstrate that for  $H_m$ , the d-dimensional tensor product of Sobolev spaces  $H_2^{(m)}[0,1]$  and  $P_{Ng}$ , the minimal norm interpolant to g at N given data points, the uniform convergence of  $\|g - P_{Ng}\|_{H_m}$  over g in the unit ball in  $H_{2m}$  cannot proceed at a rate faster than  $((\log N)^{d-1}/N)^{2m}$ . Certain conjectures concerning designs converging at this rate are made.

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## 1. Introduction.

We are interested in the problem of recovering a surface  $g(t), t \in T$ , from observations of  $g$  at a discrete set  $T_N = \{t_i\}_{i=1}^N$  of points in  $T$  (called the "design"). In particular, we are interested in choosing  $T_N$  so that an estimate, say,  $g_N$  of  $g$  from the data  $\{g(t_i)\}_{i=1}^N$  is closest to  $g$  in some appropriate sense among all designs  $T_N$ .

This problem arises in numerous applications. To cite one group of examples,  $T$  may be a sphere (the surface of the earth) or a rectangle and  $g(t)$  the 500 millibar height or the temperature, or the concentration of some air pollutant at position  $t$ . The interpolation problem requires an estimate of  $g$  over the entire surface given its values on  $T_N$  while the design problem concerns optimal or nearly optimal choices of  $T_N$ .

In this introduction we shall briefly survey several different ways of viewing the interpolation problem i.e. reconstructing the function from its sample values, and then follow this discussion with a description of some known results for the design problem in one dimension.

In this discussion of interpolation we will distinguish between the Bayesian approach and the function-analytic or deterministic approach. We further distinguish the problem of estimating  $g(t)$ , for all  $t \in T$  from estimating  $g(t)$  at a single point in  $T$  as well as introduce the possibility that our observations are distorted with errors. However, this latter feature is not primary for our objectives here.

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The Bayesian approach is as follows: We suppose  $g(t)$ ,  $t \in T$ , is a Gaussian stochastic process, or "random field" with zero mean and given strictly positive definite (prior) covariance  $K(s,t) = E g(s)g(t)$ ,  $s,t \in T$ . Given the data  $g(t_1), \dots, g(t_N)$  the Bayesian estimator for  $g(t)$  is

$$g_N(t) = E\{g(t) | g(t_1), \dots, g(t_N)\}$$

$$= (K_{t_1}(t), \dots, K_{t_N}(t)) K_N^{-1} \begin{pmatrix} g(t_1) \\ \vdots \\ g(t_N) \end{pmatrix}$$

where  $K_{t_i}(t) = K(t, t_i)$  and  $K_N$  is the  $N \times N$  matrix with  $i, j$ th entry  $K(t_i, t_j)$ , and thus

$$\min_a E(g(t) - \sum_{i=1}^N a_i g(t_i))^2$$

$$= E(g(t) - g_N(t))^2.$$

The functional analytic approach is closely related to the Bayesian approach. Instead of assuming that  $g$  is a stochastic process, suppose  $g$  is a fixed element of  $H_K$ , the reproducing kernel Hilbert space with space reproducing kernel  $K$ .

Then  $g_N$  may be shown to be the minimal norm interpolant to  $g$  on  $T_N$  in  $H_K$ , the Hilbert space with reproducing kernel  $K$ . Observing that  $\langle g, K_{t_i} \rangle_K = g(t_i)$  where  $\langle \cdot, \cdot \rangle_K$  is the inner product in  $H_K$  it can be verified that if  $P_N g$  is the minimal norm interpolator of  $g$  on  $T_N$  i.e.

$$\|P_N g\|_K = \min_{h(t_i)=g(t_i)} \|h\|_K, \quad (P_N g)(t_i) = g(t_i)$$

then  $P_N g$  is the orthogonal projection of  $g$  onto  $\text{span} \{K_{t_i}\}_{i=1}^N$  and that  $P_N g = g_N$ , see Kimeldorf and Wahba [6]. In particular,

$$(1.1) \quad \min_a E(g(t) - \sum_{j=1}^N a_j g(t_j))^2 = \min_a \|K_t - \sum_{j=1}^N a_j K_{t_j}\|_K$$

$$= \min_{a} \max_{\langle f, f \rangle_K \leq 1} |f(t) - \sum_{j=1}^N a_j f(t_j)|.$$

Minimal norm interpolation also has the striking property that it furnishes the best estimator for  $g(t)$ ,  $g \in H_K$  among *all* estimators (linear or nonlinear in  $g(t_1), \dots, g(t_N)$ ) which uses the information  $g(t_1), \dots, g(t_N)$  with  $\langle g, g \rangle_K \leq 1$ , that is,

$$\min_{A} \max_{\langle f, f \rangle_K \leq 1} |f(t) - A(f(t_1), \dots, f(t_N))|$$

where  $A$  is *any* map from  $(f(t_1), \dots, f(t_N))$  into the real line is achieved for

$A(g(t_1), \dots, g(t_N)) = g_N$ . This property and various extensions and related matters in other normed spaces is described in C.A. Micchelli and T. J. Rivlin [13].

In each instance above the data is viewed as known exactly. Frequently in applications only "noisy" data is available and this leads to the problem of data smoothing. We briefly discuss this problem in Section 5.

As a criteria for choosing  $t_1, \dots, t_N$  we minimize

$$(1.2) \quad E \int_T (g(t) - g_N(t))^2 dt = J(T_N)$$

where the expectation is taken with respect to the prior covariance  $K(s, t)$ . It is not hard to show that

$$(1.3) \quad J = J(T_N) = \int_T \{K(t, t) - (K_{t_1}(t), \dots, K_{t_N}(t)) K_N^{-1} (K_{t_1}(t), \dots, K_{t_N}(t))'\} dt.$$

In practice  $K$  may have to be estimated by use of a finer trial grid of points than will ultimately be used, or from physical principles governing the phenomena under study. The covariance of air pollution measurements for example surely depends on the local geography. If  $K$  is known, then, frequently the minimization of  $J$  will have to be carried out numerically. In this paper we will provide a lower bound for  $J$  in terms of the eigenvalues associated with the integral operator induced by  $K$ . Thus, trial solutions for the design  $T_N$  minimizing  $J$  may

be compared against the lower bound to decide whether the further minimization is worth while.

*Theorem 1. Let the operator  $K$  defined by  $(Kf)(t) = \int_T K(t,s)f(s)ds$  be a symmetric compact operator of  $L_2(T)$  into itself and have eigenvalues  $\lambda_1 \geq \lambda_2 \geq \dots$ . Then*

$$\inf_{T_N} J(T_N) \geq \sum_{i=N+1}^{\infty} \lambda_i = \int_T K(t,t)dt - \sum_{i=1}^N \lambda_i.$$

It is not known whether or not this lower bound can be achieved.

A fair amount is known about optimum designs for  $T = [0,1]$ , see Sachs and Ylvisaker [15], Wahba [19], Hajek and Kimeldorf [3]. A sequential procedure for choosing an optimum design for  $T = [0,1]$  is given in Athavale and Wahba [1]. The sequential procedure depends heavily on properties of optimal designs known from the earlier papers and does not at present generalize to  $T = [0,1] \times [0,1]$  or the sphere. In fact it appears that nothing is known about best possible convergence rates in several dimensions for  $\|g - P_N g\|_K^2$ , see Ylvisaker [21].

Sachs and Ylvisaker [16] have shown that  $\|g - P_N g\|_K^{-2}$  is the variance of the Gauss-Markov estimate of  $\theta$  in the model

$$Y(t) = \theta g(t) + X(t), \quad t \in T, \quad EX(s)X(t) = K(s,t)$$

given  $Y(t), t \in T_N$ .

If it is known that  $g$  is in some class  $C$  then it might be desirable to choose  $T_N$  to minimize  $\sup_{g \in C} \|g - P_N g\|_K^2$ . Through the notion of  $N$ -widths, introduced by Kolmogorov [7], and asymptotic estimates of the eigenvalues of certain integral operators we will provide lower bounds for the supremum of the design error for  $g$  in a certain class  $C$ . The class we will consider here is the natural generalization of the function class for which optimal one dimensional designs were obtained in [3, 15, 19]. Before stating this result we review briefly some results for optimal experimental design from [19] for  $T = [0,1]$ .



The basic assumption made in [19] about  $K$  is that it has the characteristic discontinuity of a Green's function for a  $2m$ th order self-adjoint differential operator,

$$(1.3), \quad \alpha(t) = \lim_{s \rightarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} K(s, t) - \lim_{s \rightarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} K(s, t).$$

Suppose that  $g$  has a representation

$$g(t) = \int_0^1 K(t, s) \rho(s) ds, \quad \rho \in L_2[0, 1].$$

for some  $\rho \in L_2[0, 1]$  and let  $T_N = \{t_{iN}\}_{i=1}^N$  be determined by a strictly positive density  $f$ ,

$$\int_0^{t_{iN}} f(s) ds = i/(N+1), \quad i = 1, 2, \dots, N; \quad N = 1, 2, \dots$$

Under various regularity conditions including  $\alpha, \rho > 0$

$$\begin{aligned} & \|g - P_{T_N} g\|_K^2 \\ &= \frac{C_m}{N^{2m}} \left\{ \int_0^1 \frac{\rho^2(s) \alpha(s)}{f^{(2m)}(s)} ds \right\} (1 + o(1)) \end{aligned}$$

where  $C_m$  is a constant depending on  $m$ . The density  $f$  is chosen to minimize the quantity in brackets, see [19]. Thus the rate of decay of  $\|g - P_{T_N} g\|_K^2$  is asymptotically the same as the decay of the eigenvalues of  $K$  (see Naimark [14]).

We return now to a general set  $T$  and reproducing kernel  $K$ .

**Theorem 2.** Let  $K$  be a symmetric compact operator from  $L_2(T)$  into itself with eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \dots. \text{ Let } C = \{g: g(t) = \int_T K(t, s) \rho(s) ds, \int_T \rho^2(s) ds \leq 1\}.$$

Then

$$\sup_{g \in C} \|g - P_N g\|_K^2 \geq \lambda_{N+1}$$

Next, (Section 3) we investigate the eigensequences for certain useful reproducing kernels

on  $T = \otimes^d [0, 1]$ , the tensor product of  $[0, 1]$   $d$  times. We will prove



*Theorem 3. Let  $H_K = \otimes^d H_Q$ , where  $H_Q$  is an r.k.h.s. on  $[0,1]$  with  $Q$  satisfying (1.3). Then*

$$(1.3) \quad \lambda_N = O((\log N)^{d-1}/N)^{2m}.$$

Based on this result, we make some conjectures (Section 4) concerning good designs in  $H_K$  using results from the multi-dimensional quadrature literature. In particular, we conjecture (1.3) is the optimal rate, which has only been proved for  $d=1$ , as explained above. Finally in section 5 we make some observations concerning noisy data.

## 2. Lower bounds for optimal designs.

We begin with the proof of

*Theorem 1. Let the (symmetric) operator  $K$  defined by  $(Kf)(t) = \int_T K(t,s)f(s)ds$  be compact with eigenvalues  $\lambda_1 \geq \lambda_2 \geq \dots$ . Then*

$$\inf_{T_N} J(T_N) = \inf_{T_N} \int_T \|K_t - P_N K_t\|_K^2 dt \geq \sum_{v=N+1}^{\infty} \lambda_v.$$

*Proof:* The equality is immediate from (12). Since

$$\begin{aligned} & \int_T \|K_t - P_N K_t\|_K^2 dt \\ &= \int_T \|K_t\|_K^2 dt - \int_T \|P_N K_t\|_K^2 dt \\ &= \sum_{v=1}^{\infty} \lambda_v - \int_T \|P_N K_t\|_K^2 dt, \end{aligned}$$

it suffices to show that  $\int_T \|P_N K_t\|_K^2 dt \leq \sum_{v=1}^N \lambda_v$ .

Let  $\phi_1, \dots, \phi_N$  be any  $N$  orthonormal functions in  $H_K$ . Then the projection of  $K_t$  onto span  $\{\phi_i\}_{i=1}^N$  is

$$P_N K f = \sum_{i=1}^N \phi_i(t) \phi_i,$$

and

$$\int_T \|P_N K f\|_K^2 = \sum_{i=1}^N \|\phi_i\|_{L_2}^2.$$

Let  $K^{1/2}$  be the symmetric square root of the operator  $K$ . Then by the properties of the reproducing kernel norm,

$$\|\phi_i\|_{L_2}^2 = \|K^{1/2} \phi_i\|_K^2$$

Now by the extremal properties of the eigenvalues of  $K$ ,

$$\sup_{\phi \in H_K} \|K^{1/2} \phi\|_K^2 / \|\phi\|_K^2 = \lambda_1,$$

$$\sup_{\phi \in H_K} \|K^{1/2} \phi\|_K^2 / \|\phi\|_K^2 = \lambda_2,$$

$$(\phi, \psi_1)_{L_2} = 0$$

where  $\psi_1$  is the maximizing element for the first equality above, etc. Thus,

$$\sum_{i=1}^N \|\phi_i\|_{L_2}^2 \leq \sum_{r=1}^N \lambda_r.$$

This result is also a consequence of a classical result from the theory of integral equations (see [18], 149).

**Theorem 2.** Let  $H_N$  be any  $N$  dimensional subspace in  $H_K$  and  $P_N$  be the orthogonal projection onto  $H_N$ . Then there exists a function  $g$ .

$$g(t) = \int_T K(t,s) \rho(s) ds,$$

such that

$$(2.1) \quad \|g - P_{H_N} g\|_K^2 \geq \lambda_{N+1} \int_T \rho^2(s) ds$$

Proof: The proof of this theorem also follows directly from the extremal properties for the eigenvalues of  $K^{1/2}$  and has an interpretation in the theory of N-widths, [17]. Specifically we have

$$\begin{aligned} & \inf_{H_N} \sup_{g \in C} \|g - P_{H_N} g\|_K^2 \\ &= \inf_{H_N} \sup_{\|\rho\|_{L_2}=1} \|K\rho - P_{H_N} K\rho\|_K^2 \\ &= \inf_{H_N} \sup_{\|\rho\|_{L_2}=1} \|K^{1/2}\rho - P_{H_N} K^{1/2}\rho\|_{L_2}^2. \end{aligned}$$

The extremal properties of eigenvalues and eigenfunctions of symmetric operators imply that

$$\sup_{\|\rho\|_{L_2}=1} \|K^{1/2}\rho - P_{H_N} K^{1/2}\rho\|_{L_2}^2$$

achieves its minimum for  $H_N$  equal to the span of the first N eigenfunctions of  $K^{1/2}$  and the value of the minimum is  $\lambda_{N+1}$ .

To prove the existence of an optimal design we must find a subspace of the form  $\text{span}\{K_i; i \in T_N\}$  for some design  $T_N$  which achieves the lower bound in (2.1) which would be expected to be close to the span of the first n eigenfunctions.

It should not be expected that for an arbitrary covariance kernel K an optimal design exists for each N. However, for certain classes of kernels existence of optimal designs has been shown, see Melkman [10]; Melkman and Micchelli [11].

### 3. Good designs in Tensor Product Spaces

To make use of Theorem 2 we will obtain the asymptotic rate of decay of the eigenvalues of the r.k. for  $H_K$  of the form

$$H_K = \otimes^d H_Q \text{ (tensor product of } d \text{ copies of } H_Q)$$



where  $H_Q$  is an r.k.h. s of functions on  $[0,1]$  with eigenvalues that decay as a power,

$\lambda_\nu = c\nu^{-2m}(1 + o(1)), \nu \rightarrow \infty$ . For instance, if  $Q$  behaves as a Green's function for a  $2m$ th order linear differential operator this condition is satisfied. As a simple example of this possibility, let  $H_Q = \{f: f, f', \dots, f^{(m-1)} \text{ abs. cont. } f^{(m)} \in L_2[0,1], f^{(r)}(0) = f^{(r)}(1), r = 0, 1, \dots, m-1\}$  with inner product,

$$\langle f, g \rangle = \left( \int_0^1 f(u) du \right) \left( \int_0^1 g(u) du \right) + \int_0^1 f^{(m)}(u) g^{(m)}(u) du.$$

Then the r. k.  $Q$  is

$$Q(s, t) = 1 + \sum_{\nu \neq 0} \frac{e^{2\pi i \nu(s-t)}}{(2\pi \nu)^{2m}}$$

and the corresponding eigenvalues and eigenfunctions are

$$\{1, (2\pi \nu)^{-2m}; \nu = \pm 1, \dots\}, \quad \{e^{2\pi i \nu s}; \nu = 0, \pm 1, \dots\}.$$

**Theorem 3.** Let  $H_K = \bigotimes^d H_Q$  where the eigenvalues  $\{\lambda_\nu\}$  of  $H_Q$  satisfy  $\lambda_\nu = \nu^{-2m}(1 + o(1))$  then the eigenvalues  $\{\xi_N\}$  of  $H_K$  satisfy

$$\xi_N = \left( \frac{(\log N)^{d-1}}{N} \right)^{2m} (1 + o(1))$$

**Proof.** Since  $K = \bigotimes^d Q$ , the eigenvalues of  $K$  are the tensor product of the eigenvalues of  $Q$

i.e. if  $\xi_1 \geq \xi_2 \geq \dots$  are the eigenvalues of  $K$  then

$$\{\xi_N\} = \{\lambda_{j_1} \lambda_{j_2} \dots \lambda_{j_d}; (j_1, \dots, j_d), j_1, \dots, j_d = 1, 2, \dots\}$$

To estimate the decay of  $\xi_N$  we observe that the number of lattice points  $(j_1, \dots, j_d)$  satisfying

$$\prod_{i=1}^d j_i \leq k \text{ is } k(\log k)^{d-1}(1 + o(1)).$$

Hence, since  $\lambda_\nu = \nu^{-2m}(1 + o(1))$  we have



$$\xi_{[k(\log k)^{d-1}]} = k^{-2m}(1 + o(1)).$$

([x] = greatest integer  $\leq x$ ). Choosing  $k = [N(\log N)^{d-1}]$  gives the desired conclusion,

$$\xi_N = \left( \frac{(\log N)^{d-1}}{N} \right)^{2m} (1 + o(1)).$$

It is not known for  $d > 1$  whether there exists a design for which

$$\|g - P_{N,g}\|_K^2 \leq \text{const} \left( \frac{(\log N)^{d-1}}{N} \right)^{2m} \int_{T_N} \rho^2(u) du.$$

However designs with a convergence rate approaching the optimum rate have been given in Wahba [20] for  $d=2$ .

Define

$$Z_n^j = \left\{ \frac{k}{n^j} : k = 1, \dots, n^j \right\}$$

and

$$T_{N,\ell} = \bigcup_{j=1}^{\ell+1} Z_n^j \otimes Z_n^{\ell+1-j}.$$

In [20] it is shown that  $T_{N,\ell}$  has  $N = (\ell + 1)n^{\ell+2} - \ell n^{\ell+1}$  distinct points and for

$$H_K = H_Q \otimes H_Q.$$

$$(3.1) \quad \|g - P_{T_{N,\ell}} g\|^2 \leq \text{const} \frac{(\ell+2)^2}{n^{(\ell+1)2m}} \left( \int_T \rho^2(u) du \right) (1 + o(1))$$

$$\leq \text{const} \frac{2 + \left( \frac{\ell+1}{\ell+2} \right)^{2m}}{\left( \frac{\ell+1}{\ell+2} \right)^{2m}} \left( \int_T \rho^2(u) du \right) (1 + o(1))$$

where  $g = K\rho$  and  $o(1) \rightarrow 0$  as  $n \rightarrow \infty$

Choosing  $\ell = (\log N)^p (1 + o(1))$  for any  $p$ ,  $0 < p < 1$  we have

$$N = (\ell + 1)n^{\ell+2}(1 + o(1))$$

or  $\log N = p \log \log N + (\log N)^p \log n(1 + o(1))$ . Hence

$$\log n = (1 + o(1)) \frac{\log N - p \log \log N}{(\log N)^p}$$

and  $n \rightarrow \infty$  provided  $0 < p < 1$  (for  $p=1$  this conclusion fails). Setting  $p = \frac{m}{m+1}$  into (3.1) gives

$$\|g - P_N g\|_K^2 = O\left(\frac{\left(1 + \frac{\ell+1}{\ell+2}m\right)^{/(m+1)}}{N^{\frac{\ell+1}{\ell+2}} (\log N)}\right)^{2m},$$

a convergence rate which approaches the optimum rate of  $(\log N/N)^{2m}$  implied by Theorems 2 and 3.

#### 4. Optimal quadrature - a conjecture

A quadrature formula for  $\int_T g(t) dt$  can be obtained by setting  $\int_T (P_N g)(t) dt = \sum_{i=1}^N c_i g(t_i)$ . Then

$$\begin{aligned} & \left| \int_T g(t) dt - \int_T (P_N g)(t) dt \right| \\ &= | \langle \eta, g - P_N g \rangle_K | \\ &= | \langle \eta - P_N \eta, g - P_N g \rangle_K | \\ &\leq \| \eta - P_N \eta \|_K \| g - P_N g \|_K \\ &\leq \| \eta - P_N \eta \|_K \| g \|_K \end{aligned}$$

where  $\eta$  is the representer of integration in  $H_K$ ,

$$\eta(s) = \langle \eta, K_s \rangle_K = \int_T K(s, u) du$$

An optimal quadrature problem may be formulated as: Find  $t_1, \dots, t_N$  to minimize

$$\| \eta - P_N \eta \|_K.$$

There is a large literature on choosing sequences in the  $d$ -dimensional unit cube which makes the error for the special quadrature formula  $\frac{1}{N} \sum_{i=1}^N g(t_i)$  asymptotically small. This work has focused on finding sequences  $T_N = \{t_1, \dots, t_N\}$  for which the discrepancy  $D_N$  defined by

$$D_N = \sup_i |F_N(t) - F(t)|$$

is small. Here  $F_N$  is the cumulative distribution function of the point set and  $F$  is the cumulative distribution of the uniform density, see Kuipers and Neiderreiter [8], Halton [4], Halton and Zaremba [5], Zaremba [22].

It is known that the Hammersly sequences defined below, have discrepancy

$$D_N = \left( \frac{\log^{d-1} N}{N} \right) (1 + o(1))$$

see Halton [4].

These sequences are defined (in d-dimensions) by

$$\left\{ \frac{n}{N}, \phi_2(n), \phi_3(n), \dots, \phi_d(n) \right\}_{n=0}^{N-1}$$

where the subscripts in the  $\phi$ 's are successive primes and if  $n = \sum_{j=0}^M n_j p^j$  where  $M = [\log_p n]$ ,

$$\text{then } \phi_p(n) = \sum_{j=1}^{M+1} n_j p^{-j}.$$

$$\text{Bounds on } \epsilon_N = \left| \int_T g(t) dt - \frac{1}{N} \sum_{i=1}^N g(t_i) \right|$$

in terms of the discrepancy appear in the literature, see Kuipers and Neiderreiter [8, p. 157], Zaremba [22] and references therein.

In [8] it is shown for certain sequences that  $\epsilon_N = O(D_N^q)$  where  $g$  has

Fourier coefficients  $c_{r_1, r_2, \dots, r_d}$  satisfying

$$|c_{r_1, r_2, \dots, r_d}| \leq \frac{M}{\left( \prod_{i=1}^d \bar{r}_i \right)^q}$$

where

$$\bar{r}_i = \begin{cases} |r_i| & r_i \neq 0 \\ 1 & r_i = 0 \end{cases}.$$



We conjecture that similar results obtain for Hammersley sequences and that for spaces  $H_K$  satisfying the hypothesis of Theorem 2 the optimal convergence rate

$$\|g - P_N g\|_K^2 = \lambda_{N+1}(1 + o(1)) \\ = \left(\frac{(\log N)^{d-1}}{N}\right)^{2m}(1 + o(1))$$

will hold for  $T_N$  the Hammersley sequence and  $g$  of the form  $g = K\rho$ .

### 5. Noisy Data

In this section we include some remarks concerning estimation based on inaccurate data.

If instead of observing  $g(t), t \in T_N$ , we assume that the data is given by

$$y_i = g(t_i) + \epsilon_i, \quad E\epsilon_i\epsilon_j = \delta_{ij}.$$

then the minimum norm estimator

$$\min_a E(g(t) - \sum_{i=1}^N a_i y_i)^2 = \|K_t - \sum_{j=1}^N a_j K_{t_j}\|_K^2 + \sigma^2 \sum_{j=1}^N a_j^2$$

leads in the functional-analytical approach to

$$(5.1) \quad = \min_a \max_{\langle f, f \rangle_K \leq 1} |f(t) - \sum_{i=1}^N a_i f(t_i)|^2 + \sigma^2 \sum_{i=1}^N a_i^2$$

Recently, this variational problem has been solved by Laurent [9]. It has been shown that the minimum norm estimator is the smoothing "spline" in  $H_K$  with parameter  $\sigma^{-2}$ , that is, if  $g_N$  minimizes

$$(5.2) \quad \min \{ \|f\|_K^2 + \sigma^{-2} \sum_{i=1}^N (f(t_i) - g(t_i))^2 \}$$

then  $g_N(t) = \sum_{i=1}^N c_i(t)g(t_i)$  is the minimum norm estimator for  $g$  when we have noisy data.

Note that the smoothing parameter  $\sigma^2$  does *not* depend on the value  $t \in T$  at which we choose to estimate  $g(t)$ . The following short proof of this result is instructive: We wish to determine



$$\min_a \left\| K_t - \sum_{i=1}^N a_i K_{t_i} \right\|_K^2 + \sigma^2 \sum_{j=1}^N a_j^2$$

To this end, we introduce the tensor product space  $H_K \otimes R^N = \{(f, a) \mid f \in H_K, a \in R^N\}$  with the norm

$$\|(g, a)\|_o^2 = \|g\|_K^2 + \sigma^2 \sum_{i=1}^N a_i^2$$

Then the above problem in  $H_K \otimes R^N$  becomes

$$\min_a \left\| h - \sum_{j=1}^N a_j h_j \right\|_o$$

$$h = (K_t, 0), \quad h_j = (K_{t_j}, -e_j) \quad (e_j)_k = \delta_{jk}.$$

But from the theory for estimating exactly given data, as in (1.1), the minimum  $a = (a_1, \dots, a_N)$  may be obtained from the best interpolant,

$$\begin{aligned} \min_{(f, a), (K_{t_i}, -e_i) \in g(t_i)} \|(f, a)\|_o^2 = \\ \min_f \left\{ \|f\|_K^2 + \sigma^{-2} \sum_{i=1}^N (g(t_i) - f(t_i))^2 \right\} \end{aligned}$$

in agreement with (5.2).

It has not yet been determined if the optimality of smoothing "splines" persists when an estimator for the full function  $g(t)$ ,  $t \in T$  when the error criteria (1.2) is used. However, let us replace (5.1) by

$$\min_a \max_{\substack{\langle f, f \rangle \leq 1 \\ \sum_{i=1}^N r_i^2 \leq 1}} \left| f(t) - \sum_{i=1}^N a_i (f(t_i) + \epsilon r_i) \right|^2$$

that is, we minimize the worst least square error when we know the noise in the data is in the region  $y_i = f(t_i) + \epsilon r_i$ ,  $\sum_{i=1}^N r_i^2 \leq 1$ . It has been shown that in this setting the smoothing spline is also optimal. However, unlike (5.1), the smoothing parameter depends on  $\epsilon$  as well as  $t \in T$ . Moreover, this theory holds in great generality, including, in particular, estimating the full function  $g(t)$ ,  $t \in T$  (see Melkman and Micchelli [13] for the details). For methods of

choosing the smoothing parameter using a cross-validation procedure based on the data see Craven and Wahba [2].

The design problem of Theorem 1, has an analogue for noisy data which may be described as follows. Let  $g(t)$ ,  $t \in T$  be a stochastic process as before and let  $g_N(t) =$

$$E\{g(t) | y_1, \dots, y_N\} = (K_{t_1}(t), \dots, K_{t_N}(t))(K_N + \sigma^2 I)^{-1}(y_1, \dots, y_N)'.$$

Then  $J_N$  becomes

$$\begin{aligned} J_N &= E \int_T (g(t) - g_N(t))^2 dt \\ &= \int_T \{K(t, t) - (K_{t_1}(t), \dots, K_{t_N}(t))(K_N + \sigma^2 I)^{-1}(K_{t_1}(t), \dots, K_{t_N}(t))'\} dt. \end{aligned}$$

which may be compared to equation (1.2).

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Using minimal norm interpolation in reproducing kernel Hilbert spaces, equivalently Bayesian interpolation, and N-widths, we provide lower bounds for interpolation error relative to certain error criteria. These lower bounds can be used when evaluating an existing design, or when attempting to obtain a good design by iterative procedures to decide whether further minimization is worthwhile. The bounds are given in terms of the eigenvalues of a relevant reproducing kernel and the asymptotic behavior of these eigenvalues for certain tensor product spaces in the unit d-dimensional cube is obtained.

We demonstrate that for  $H_m$ , the d-dimensional tensor product of Sobolev spaces  $W_2^{(m)}[0,1]$  and  $P_{Ng}$ , the minimal norm interpolant to g at N given data points, the uniform convergence of  $\|g - P_{Ng}\|_{H_m}$  over g in the unit ball in  $H_{2m}$  cannot proceed at a rate faster than  $((\log N)^{d-1}/N)$ . Certain conjectures concerning designs converging at this rate are made.

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